SELECTIVE SORBENTS FOR PURIFICATION OF HYDROCARBONS

ABSTRACT OF THE DISCLOSURE

CuY and AgY zeolites as selective sorbents for desulfurization of liquid fuels. Thiophene and benzene were used as the model system, and vapor phase isotherms were measured. Compared with NaY, CuY and AgY adsorbed significantly larger amounts of both thiophene and benzene at low pressures. It is hypothesized that this is due to π -complexation with Cu^+ and Ag^+. On a per-cation basis, more thiophene was adsorbed by Cu^+ than by Ag^+, e.g., 0.92 molecule/Cu^+ versus 0.42 molecule/Ag^+ at $2x10^{-5}$ atm and 120°C. Molecular orbital calculations confirmed the relative strengths of π-complexation: thiophene > benzene and $Cu^+ > Ag^+$. The experimental heats of adsorption for π-complexation are in qualitative agreement with theoretical predictions. The invention further comprises a process and sorbents for removal of aromatics from hydrocarbons.

Fixed-bed adsorption using π-complexation adsorbents for desulfurization of commercial liquid fuels was investigated. Cu(I)-Y (auto-reduced Cu(II)-Y) zeolites were used to separate low concentration sulfur molecules from commercial gasoline and diesel samples, all at room temperature and atmospheric pressure. Sulfur-free fuels were obtained with Cu(I)-Y and a combination of activated carbon (AC) and Cu(I)-Y. Activated carbon was used as a guard bed. Breakthrough and saturation adsorption capacities obtained for an influent average total concentration of 335 ppmw sulfur in gasoline showed that Cu(I)-Y is capable of processing 14.7 cm^3 of sulfur free gasoline per gram of adsorbent and remove 1.4 wt% sulfur at saturation. When using activated carbon as a guard bed with Cu(I)-Y zeolite, the combination is capable of processing 19.6 cm^3 of sulfur free gasoline per gram of adsorbent. For the case of diesel fuel, AC/Cu(I)-Y adsorbed 1.08 and 1.85 wt% total sulfur at breakthrough and saturation, respectively. At breakthrough, the adsorbent plus guard bed is capable of processing 34.3 cm^3 of sulfur free diesel per gram of adsorbent. GC-FPD data reveals the π-complexation adsorbents are capable of removing heavily substituted thiophenes, benzothiophenes, and dibenzothiophenes, which is not possible using conventional Hydrodesulfurization (HDS) reactors. FTIR data supports that a low concentration of aromatics in untreated fuels is beneficial for the removal of sulfur species.